Wide-angle split-step spectral method for 2D or 3D beam propagation

C. D. Clark III · Robert J. Thomas

Abstract We develop a method for non-paraxial beam propagation that obtains a speed improvement over the Finite-Difference Split-Step method (FDSSNP) recently reported by Sharma et al. The method works in the eigen-basis of the Laplace operator $\left(\nabla_T^2\right)$, and in general requires half as many operations to propagate one step forward so that a 2X speedup can be realized. However, the new formulation allows the Fast Fourier Transform (FFT) algorithm to be used, which allows an even greater speedup. The method does not require a numerical matrix inversion, diagonalization, or series evaluation. The diffraction operator is not approximated, and in the absence of refractive index fluctuations the method reduces to an exact solution of the Helmholtz equation.

Keywords Beam propagation · Spectral · Wide-angle

1 Introduction

Beam propagation methods (BPM) are a large class of numerical methods for solving the scalar Helmoltz equation. They are popular for simulating guided waves and laser beams, as they are typically both fast and efficient. Early methods used the paraxial approximation, which greatly simplified the problem by reducing the propagation equation to first order, but they were severely limited in their application because any beam profile containing spacial frequencies with angles greater than a few degrees with respect to the propagation axis incur significant phase errors. Many methods were developed to drop the paraxial approximation and include wide-angle waves. In several of these, the Helmholtz equation is formally rewritten as a first-order differential equation which includes the square root of an

C. D. Clark III (✉)
TASC, Inc., 2624 Louis Bauer Drive, Brooks City-Base, TX 78235, USA
e-mail: clifton.clark.ctr@brooks.af.mil

R. J. Thomas
AFRL 711/HPW RHDO, 2624 Louis Bauer Drive, Brooks City-Base, TX 78235, USA
e-mail: robert.thomas@brooks.af.mil

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operator. Then the square root operator is either approximated using real or complex Padé approximants and a Finite-Difference or iterative method is used to solve the equation (Hadley 1992; Le et al. 2008), or the formal solution is written which results in an exponential of the square root of an operator that is then approximated with a Padé approximant (Lu and Ho 2002).

Recently, Sharma extended an operator-splitting technique used on the paraxial wave equation to the non-paraxial wave equation (Helmholtz equation) Sharma and Agrawal (2004). The splitting allows diffraction and the refractive index variations to be handled separately, and various numerical methods can be used after the operator has been split, such as collocation or Finite-Differencing (Sharma and Agrawal 2004, 2006). Here we develop a method that represents the beam profile in the eigenbasis of the diffraction operator and uses the operator-splitting technique to account for the refractive index variations. In general, the method provides a 2X speedup to the Finite-Difference method reported by Sharma, but this can be increased by use of the Fast Fourier Transform algorithm.

2 Formulation

Beam propagation in a non-uniform refractive index distribution is described by the Scalar Wave Equation,

$$\frac{\partial^2}{\partial z^2}\Psi\left(z,\mathbf{x}\right) + \nabla_T^2\Psi\left(\mathbf{x}\right) + k_0^2\bar{n}^2\Psi\left(z,\mathbf{x}\right) + k_0^2\left(n^2\left(z,\mathbf{x}\right) - \bar{n}^2\right)\Psi\left(z,\mathbf{x}\right) = 0. \qquad (1)$$

Here, $\Psi\left(z,\mathbf{x}\right)$ is the scalar electric field given in two or three dimensions and ∇_T^2 is the one or two dimensional transverse part of the Laplacian. As usual, k_0 denotes the free-space wave-number of the beam, $n^2\left(z,\mathbf{x}\right)$ is the refractive index of the medium and $\bar{n}^2$ is a background refractive index, usually taken to be $\min\left\{n^2\left(z,\mathbf{x}\right)\right\}$. The term $\left(n^2\left(z,\mathbf{x}\right) - \bar{n}^2\right)$ can be viewed as a perturbation to the homogeneous propagation in a media with refractive index $\bar{n}$. Consider the set of eigenfunctions $\left(\phi_n\left(\mathbf{x}\right)\right)$ and eigenvalues $\left(-\lambda_n^2\right)$ of the transverse Laplacian satisfying the waveguide boundary condition. They are defined as

$$\nabla_T^2\phi_n\left(\mathbf{x}\right) = -\lambda_n^2\phi_n\left(\mathbf{x}\right),$$
$$\int \phi_n^*\left(\mathbf{x}\right)\phi_m\left(\mathbf{x}\right)d\mathbf{x} = \delta_{n,m}, \qquad (2)$$
$$\phi_n\left(\mathbf{X}\right) = 0,$$

where $\mathbf{X}$ is the coordinate of the waveguide wall. The eigenfunctions form a complete basis, so we expand the field profile

$$\Psi\left(z,\mathbf{x}\right) = \sum_{n=1}^{\infty} a_n\left(z\right)\phi_n\left(\mathbf{x}\right). \qquad (3)$$

Inserting 3 into Eq. 1, then multiplying by $\phi_m^*\left(\mathbf{x}\right)$ and integrating gives a system of differential equations,

$$\frac{\partial^2}{\partial z^2}a_m\left(z\right) = -\left(k_0^2\bar{n}^2 - \lambda_m^2\right)a_m\left(z\right) - \sum_{n=1}^{\infty}\int k_0^2\left(n^2\left(z,\mathbf{x}\right) - \bar{n}^2\right)\phi_m^*\left(\mathbf{x}\right)\phi_n\left(\mathbf{x}\right)d\mathbf{x}\, a_n\left(z\right).$$

$$(4)$$

The eigenfunction profiles, ϕ_n, are propagating modes, and Eq. 4 is the set of equations that govern the mode amplitudes. If the refractive index were constant, i.e. $n^2(z, \mathbf{x}) - \bar{n}^2 = 0$, then the modes would each propagate independent of the others. However, the last term of Eq. 4 couples these modes, allowing energy to transfer between them. Note also that this term is just the refractive index operator (which is diagonal in the spatial coordinates) represented in the basis of eigenfunctions, and can be written in operator form as $\mathbb{S} \mathbb{N}(z) \mathbb{S}^{-1} \mathbf{a}$.

We now proceed to implement the split-step method described by Sharma and Agrawal (2004, 2006), Sharma et al. (2007). Equation 4 can be written in matrix form,

$$b_m = \partial_z a_m,$$
$$A = \begin{bmatrix} a_m \\ b_m \end{bmatrix}, \quad \mathbb{H}(z) = \begin{bmatrix} 0 & \mathbb{I} \\ -\left(k_0^2 \bar{n}^2 - \lambda_m^2\right)\mathbb{I} - \mathbb{S} \mathbb{N}(z) \mathbb{S}^{-1} & 0 \end{bmatrix}, \quad (5)$$
$$\partial_z A = \mathbb{H}(z) A,$$

which has the solution $A(z_0 + \Delta z) = e^{\mathbb{H}(z)\Delta z} A(z_0)$. The operator $\mathbb{H}(z)$ can be written as the sum of two operators,

$$\mathbb{H}(z) = \mathbb{H}_1 + \mathbb{H}_2(z), \quad (6)$$

$$\mathbb{H}_1 = \begin{bmatrix} 0 & \mathbb{I} \\ -\left(k_0^2 \bar{n}^2 - \lambda_m^2\right)\mathbb{I} & 0 \end{bmatrix}, \quad (7)$$

$$\mathbb{H}_2(z) = \begin{bmatrix} 0 & 0 \\ -\mathbb{S} \mathbb{N}(z) \mathbb{S}^{-1} & 0 \end{bmatrix}, \quad (8)$$

so that

$$A(z_0 + \Delta z) = e^{(\mathbb{H}_2 + \mathbb{H}_2(z))\Delta z} A(z_0). \quad (9)$$

The matrix exponential cannot simply be split into the product of two matrix exponentials because the matrices $\mathbb{H}_1$ and $\mathbb{H}_2(z)$ do not in general commute. Instead, the exponential is approximated using a symmetrized operator splitting technique (Sharma and Agrawal 2004, 2006; Dattoli et al. 1998),

$$e^{\mathbb{H}(z)\Delta z} \approx e^{\frac{1}{2}\mathbb{H}_1\Delta z} e^{\mathbb{H}_2(z)\Delta z} e^{\frac{1}{2}\mathbb{H}_1\Delta z} \quad (10)$$

which is second-order accurate in Δz (Sharma and Agrawal 2004, 2006; Dattoli et al. 1998; Fleck et al. 1976). It is clear that $e^{\frac{1}{2}\mathbb{H}_1\Delta z}$ propagates the mode a half step forward in a uniform media, so $e^{\mathbb{H}_2(z)\Delta z}$ must account for the inhomogeneous refractive index.

The next step is to compute the two matrix exponentials. Expanding the exponential in its power series form and evaluating the sum gives (Sharma and Agrawal 2006; Sharma et al. 2007),

$$e^{\mathbb{H}_2(z)\Delta z} = \mathbb{Q} = \begin{bmatrix} \mathbb{I} & 0 \\ -\mathbb{S} \mathbb{N}(z) \mathbb{S}^{-1}\Delta z & \mathbb{I} \end{bmatrix}, \quad (11)$$

$$e^{\frac{1}{2}\mathbb{H}_1\Delta z} = \mathbb{P} \quad (12)$$

$$= \begin{bmatrix} \cos\left(\sqrt{k_{z,m}^2\mathbb{I}}\Delta z/2\right) & \sin\left(\sqrt{k_{z,m}^2\mathbb{I}}\Delta z/2\right)/\sqrt{k_{z,m}^2\mathbb{I}} \\ -\sqrt{k_{z,m}^2\mathbb{I}}\sin\left(\sqrt{k_{z,m}^2\mathbb{I}}\Delta z/2\right) & \cos\left(\sqrt{k_{z,m}^2\mathbb{I}}\Delta z/2\right) \end{bmatrix}. \quad (13)$$

where we have used $k_{z,m}^2 = \left(k_0^2 \bar{n}^2 - \lambda_m^2\right)$. The difference between this and the Finite-Difference formulation is that the operators under the square root are already diagonal,

Table 1 Application to various coordinate systems

2D, Cartesian coordinates $\left(\partial_y^2 \Psi = 0\right)$

$\nabla_T^2 \rightarrow \frac{\partial^2}{\partial x^2}$

$\mathbb{S} \rightarrow$ Sine Transform

$\phi\left(\mathbf{x}\right) \rightarrow \sin\left(k_n x\right)$

$-\lambda^2 \rightarrow -k_n^2$

$k_n \rightarrow \frac{n\pi}{X}$

2D, Cylindrical coordinates $\left(\partial_\phi^2 \Psi = 0\right)$

$\nabla_T^2 \rightarrow \frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}$

$\mathbb{S} \rightarrow$ Hankel Transform

$\phi\left(\mathbf{x}\right) \rightarrow J_0\left(\rho_n r\right)$

$-\lambda^2 \rightarrow -\rho_n^2$

$\rho_n \rightarrow \frac{\alpha_n}{R}$

3D, Cartesian coordinates

$\nabla_T^2 \rightarrow \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$

$\mathbb{S} \rightarrow$ 2D Sine Transform

$\phi\left(\mathbf{x}\right) \rightarrow \sin\left(k_n x\right)\sin\left(k_m y\right)$

$-\lambda^2 \rightarrow -\left(k_n^2 + k_m^2\right)$

$k_n \rightarrow \frac{n\pi}{X}$

$k_m \rightarrow \frac{m\pi}{Y}$

so they can be directly evaluated. These two matrices can be used to propagate an initial A forward one step in the z direction. The complete propagation algorithm is then written as

$$A(z_0 + n\Delta z) = \mathbb{P}\mathbb{Q}\left(z_0 + (n-1)\Delta z\right)\mathbb{P}\cdots\mathbb{P}\mathbb{Q}\left(z_0 + \Delta z\right)\mathbb{P}\mathbb{P}\mathbb{Q}\left(z_0\right)\mathbb{P}A\left(z_0\right).$$

However, we note that since $[\mathbb{H}_1, \mathbb{H}_1] = 0$,

$$e^{\frac{1}{2}\mathbb{H}_1\Delta z}e^{\frac{1}{2}\mathbb{H}_1\Delta z} = e^{\mathbb{H}_1\Delta z}$$

$$\mathbb{P}\mathbb{P} = \begin{bmatrix} \cos\left(\sqrt{k_{z,m}^2}\Delta z\right) & \sin\left(\sqrt{k_{z,m}^2}\Delta z\right)/\sqrt{k_{z,m}^2} \\ -\sqrt{k_{z,m}^2}\sin\left(\sqrt{k_{z,m}^2}\Delta z\right) & \cos\left(\sqrt{k_{z,m}^2}\Delta z\right) \end{bmatrix}.$$

So far, the derivation of the propagation algorithm has not depended on the eigenfunctions ϕ_n, only their properties (Eq. 2). This is convenient because the method is independent of the specific coordinate system used (only that it is rectilinear in z). Choosing a coordinate system then sets the eigenfunctions which defines $\mathbb{S}$ and the eigenvalues, $-\lambda^2$ (See Table 1). In principle, any coordinate system could be used, as long as a numerical representation of the associated eigenfunction basis transform is available.

3 Numerical example

To test the method, and compare it to Sharma's FDSSNP method, we have simulated propagation through the 2-dimensional (Cartesian) symmetric *Epstein-layer* waveguide, whose refractive index profile is given as

Table 2 Test case configuration

$$n^2(x, z) = \bar{n}^2 + 2\bar{n}\Delta n \operatorname{sech}^2\left(2\left(x\cos\theta - z\sin\theta\right)/w\right)$$

$$\bar{n} = 2.1455$$

$$\Delta n = 0.003$$

$$w = 5\,\mu\text{m}$$

$$\lambda_0 = 1.3\,\mu\text{m}$$

$$\theta = 0°,\ 50°$$

$$n^2(x) = \bar{n}^2 + 2\bar{n}\Delta n \operatorname{sech}^2(2x/w). \tag{14}$$

Table 2 lists the specific values used in the configuration. The zero'th order mode is

$$\Psi_0(x, 0) = \operatorname{sech}^W(2x/w),$$

$$\Psi_0(x, z) = \Psi_0(x, 0)\,e^{ik_{z0}z},$$

$$W = \frac{1}{2}\left(\sqrt{1 + 4\left(\frac{\pi^2 w^2}{\lambda_0^2}\right)2\bar{n}\Delta n} - 1\right),$$

$$k_{z0} = \sqrt{W^2 + \left(\frac{2\pi\bar{n}}{\lambda_0}\right)^2}.$$

If the waveguide is rotated such that it makes an angle θ with the z-axis, the refractive index and field become

$$n^2(x, z) = \bar{n}^2 + 2\bar{n}\Delta n \operatorname{sech}^2\left(2\left(x\cos\theta - z\sin\theta\right)/w\right),$$

$$\Psi_0(x, 0) = \operatorname{sech}^W\left(2\left(x\cos\theta\right)/w\right)e^{ik_{z0}x\sin\theta},$$

$$\Psi_0(x, z) = \Psi_0(x, 0)\,e^{ik_{z0}z\cos\theta}.$$

We use the *correlation factor* to measure error,

$$CF(z) = \frac{\left|\int \Psi_0^*(x, z)\,\psi_0(x, z)\,dx\right|^2}{\left|\int \Psi_0^*(x, z)\,\Psi_0(x, z)\,dx\right|^2},$$

$$ERR(z) = 1 - CF(z),$$

where Ψ_0 is the exact beam profile and ψ is the computed profile, as it provides a measure for both the profile shape and amplitude (Sharma and Agrawal 2006).

We have implemented C++ versions of both the FDSSNP and our method. The programs were compiled with g++, version 4.4.3, and all simulations where ran on an Intel Core 2 Duo, 2.66 GHz processor with 8 GB of RAM.

The eigenfunctions of the transverse Laplace are harmonic sine functions. The transform, $\mathbb{S}$, is a Sine Transform, and can be applied with an FFT library. We used the FFTW library, version 3.2.2. Figures 1 and 2 show the error with propagation distance for an aligned and rotated waveguide for various values of Δz and demonstrate the algorithm's stability.

The sub-matrices of $\mathbb{PP}$ in the Finite-Difference representation are, in general, dense. To reduce the number of operations needing during the propagation steps, the sub-matrices are precomputed. We have used the BLAS library to apply $\mathbb{PP}$, which is known to be very efficient and fast. Our Spectral method is shown to be about twice as fast for the smallest transverse grid we tested, 300 points, but over 10 times faster for the large grid, 1200 points (Fig. 3).
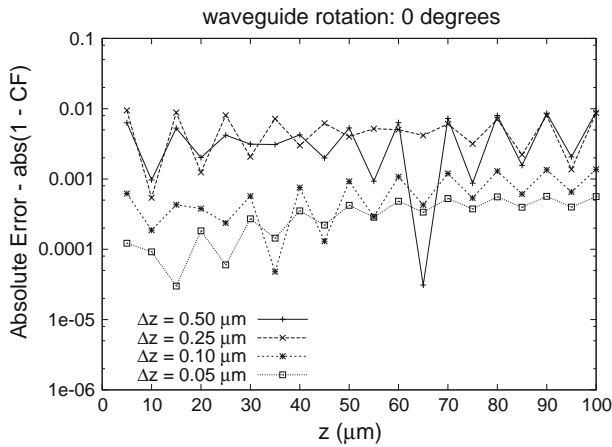
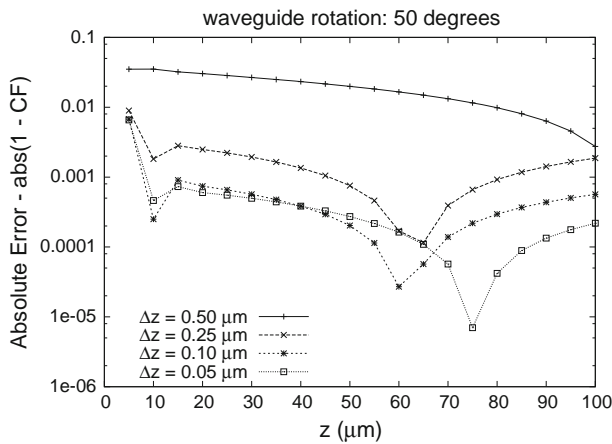**Fig. 1** Error as a function of propagation distance for aligned waveguide

Fig. 2 Error as a function of propagation distance for waveguide tilted at 50 degrees

4 Discussion

4.1 Speedup

The reason for the observed speedup of our Spectral method follows directly from the form of $\mathbb{P}$ and $\mathbb{Q}$. In the Finite-Difference method, $\mathbb{P}$ and $\mathbb{Q}$ are represented as (Sharma et al. 2007),

$$\mathbb{Q} = \begin{bmatrix} \mathbb{I} & 0 \\ -\mathbb{N}(z)\,\Delta z & \mathbb{I} \end{bmatrix}, \tag{15}$$

$$\mathbb{P} = \begin{bmatrix} \mathbb{V}\left[\cos\left(\sqrt{\mathbb{K}}\Delta z/2\right)\right]\mathbb{V} & \mathbb{V}\left[\sin\left(\sqrt{\mathbb{K}}\Delta z/2\right)/\sqrt{\mathbb{K}}\right]\mathbb{V} \\ -\mathbb{V}\left[\sqrt{\mathbb{K}}\sin\left(\sqrt{\mathbb{K}}\Delta z/2\right)\right]\mathbb{V} & \mathbb{V}\left[\cos\left(\sqrt{\mathbb{K}}\Delta z/2\right)\right]\mathbb{V} \end{bmatrix}, \tag{16}$$

where $\mathbb{K}$ is the diagonal matrix constructed using the series representation of the Finite-Difference operator, and $\mathbb{V}$ is the matrix that diagonalizes the Central-Difference operator.
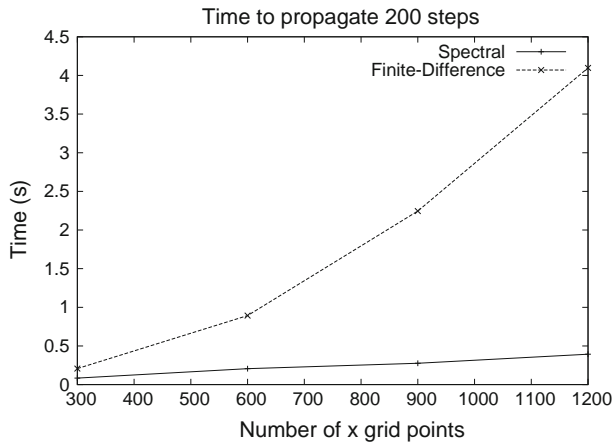
Fig. 3 A comparison of the time required to propagate 200 steps for the Finite-Difference method and our Spectral method for various transverse grid resolutions

As more terms are used to construct $\mathbb{K}$, $\mathbb{P}$ becomes increasingly dense, and so in general, $\mathbb{P}$ is composed of four $N_T \times N_T$ matrices.[1] The matrix $\mathbb{Q}$ is composed of three diagonal matrices, but only one needs to be explicitly applied. Application of $\mathbb{PQ}$ (or $\mathbb{PPQ}$) requires one vector-vector element-wise product and four matrix-vector multiplications with a complex input vector, so a total of $2\left(4N_T^2 + N_T\right)$ multiplications are required.

The form of $\mathbb{P}$ and $\mathbb{Q}$ derived here only require $2\left(5N_T + 2N_T^2\right)$ multiplications to be applied. $\mathbb{P}$ is composed of four diagonal matrices, which requires four vector-vector element-wise products. $\mathbb{Q}$ only contains one matrix that must be applied, but it is applied using one matrix-vector multiplication followed by a vector-vector element-wise product and another matrix-vector multiplication. So in general, the Finite-Difference method requires $\frac{4N_T+1}{2N_T+5}$ times, or roughly 2 times, as many multiplications as our Spectral method. However, as noted above, in Cartesian coordinates, the transformation matrix $\mathbb{S}$ can be applied using an FFT library, which can apply $\mathbb{S}$ in about $N_T \log N_T$ multiplications. For such cases, the Finite-Difference method will require $\frac{4N_T+1}{2\log N_T+5}$ more multiplications, which leads to significant speed improvements as N_T gets large.

4.2 Other coordinate systems

Both the Finite-Difference and Spectral formulations can be be applied to multiple coordinate systems. The Finite-Difference approach requires a Finite-Difference representation of ∇_T^2 that must then be diagonalized numerically or analytically, whereas the Spectral approach requires numerical representations of the eigenfunction transforms associated with ∇_T^2. Sharma has recently shown that the Finite-Difference approximation of ∇_T^2 in 2D Cartesian coordinates ($\nabla_T^2 \rightarrow \partial_x^2$) (Sharma et al. 2007) and 3D Cartesian coordinates ($\nabla_T^2 \rightarrow \partial_x^2 + \partial_y^2$) (Bhattacharya and Sharma 2007) can be diagonalized analytically. Nash has shown similarly that the Finite-Difference approximation of ∇_T^2 in 2D Cylindrical coordinates ($\nabla_T^2 \rightarrow r^{-1}\partial_r r \partial_r$) (Nash and López-Mobilia 2004) can also be diagonalized analytically, which could be used to formulate a Finite-Difference based split-step propagation method in systems possessing azimuthal symmetry.

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[1] Here, N_T denotes the number of transverse grid points.

As outlined in Table 1, in the Spectral method formulation, these coordinate systems require 1D and 2D Fourier Transforms which can be computed using FFT libraries (Press et al. 2002) and a Hankel Transform, which could be computed using the Quasi-Discrete Hankel Transform (Yu et al. 1998; Guizar-Sicairos and Gutié 2004) for example.

4.3 Boundary conditions

We have assumed the boundary condition $\phi_n (\mathbf{X}) = 0$ for each of the eigenfunctions, which imposes the "hard wall" boundary condition on the field; the computational domain is surrounded by a perfectly reflecting metal surface. This can be a serious problem, especially when simulating photonic devices, because it prevents energy loss through the radiation modes as any wave reaching the boundary will be reflected back into the waveguide. However, for applications in beam propagation, this is typically not an issue because the beam profile will have a finite size and the hard wall boundary can be placed far enough away such that it does not interfere with the beam.

It would also be possible to implement non-reflecting boundary conditions, such as the Perfectly Matched Layer (PML), although our applications have so far not required this. Multiple non-reflecting boundary conditions have been developed for the Eigen Mode Expansion method (EME) (Bienstman and Baets 2002), and the same methods could be applied here. For example, a PML can derived by simply considering the layer to have a complex thickness (Bienstman and Baets 2001; Derudder et al. 2001). To add a PML, a layer with an imaginary component to its space coordinate would be placed before the hard wall, to absorb all incident waves. The general eigenfunctions (and eigenvalues) of ∇_T^2 would then need to be found for this geometry to construct the basis transformation, $\mathbb{S}$, and the propagation algorithm would remain unchanged.

However, the change in basis functions to include a PML would mean that the FFT algorithm could not be used, and only a 2X speedup over the FDSSNP method could be achieved. The use of a non-reflective boundary condition would most likely only be beneficial when boundary interference cannot be avoided by placing the metal surface farther away, or the coordinate system does not allow use of the FFT (such as cylindrical coordinates). For example, transforming a vector of 400 points using a full matrix-vector multiplication costs approximately the same computational time as transforming a vector of 35,000 points using the FFT. So the computational domain could be made over 80 times larger using the FFT, before the matrix-vector multiplication became more efficient.

5 Conclusions

We have outlined a method here that improves the performance of the wide-angle split-step beam propagation method recently developed by Sharma. The method recasts the propagation equation into the Spectral domain of the transverse Laplacian operator and depends on numerical representations of special function transforms, rather than Finite-Difference representations of the transverse Laplacian. The method requires roughly half as many floating point multiplications as the Finite-Difference method in general because of the particular operator splitting used to approximate the operator exponential, the FFT can be used to reduce this further. We have demonstrated the algorithm in 2D Cartesian coordinates, but the method derived here is equally applicable to 2 and 3D beam propagation in Cartesian or Cylindrical coordinates, and the numerical transforms needed for both cases are available in the literature.

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